2. (Quantum Mechanics)

A spin-1/2 particle of mass m is restricted to move in the x-direction only. It moves in a potential whose x dependence is that of an infinite square well of width $2L$

$$V(x) = \begin{cases} 0 & -L \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$$

The particle also couples to a magnetic field via a term in the Hamiltonian $H_B = \mu_0 \boldsymbol{\sigma} \cdot \mathbf{B}$, where σ_i are the Pauli matrices. The magnetic field takes the form

$$\mathbf{B} = \begin{cases} B\,\hat{\mathbf{z}} & -L \leq x \leq 0 \\ B\,\hat{\mathbf{x}} & 0 < x \leq L \end{cases} \tag{68}$$

What are the energy levels of the particle to first order in B?

Solution: *Solution by Jonah Hyman (jthyman@g.ucla.edu)*

This problem concerns the one-dimensional particle in a box (infinite square well potential). Here is what you need to know about the particle in a box for this problem:

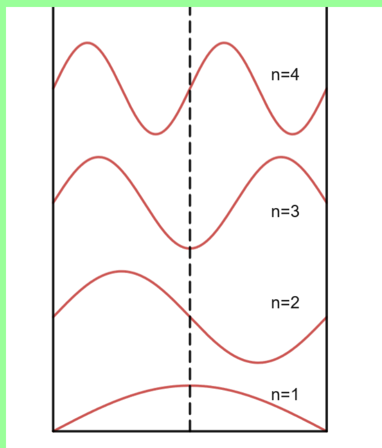
One-dimensional particle in a box (infinite square well potential)
For a particle in a one-dimensional box of length a, the energy eigenfunctions of the particle consist of sines and cosines that are equal to zero at both sides of the box, i.e., that have allowed wavenumbers

$$k_n = \frac{n\pi}{a} \quad \text{for} \quad n = 1, 2, 3, \ldots \tag{69}$$

The eigenenergies are then given by

$$E_n = \frac{p_n^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \quad \text{for} \quad n = 1, 2, 3, \ldots \tag{70}$$

Here is a graph of the first few eigenfunctions. Note that for n odd, the eigenfunctions are even functions, as measured about the center of the box. For n even, the eigenfunctions are odd functions, as measured about the center of the box.



The problem is a first-order degenerate time-independent perturbation theory problem: Even though the one-dimensional particle in a box has nondegenerate energy levels E_n, the addition of the particle's spin creates a degeneracy since the infinite square well potential does not depend on the spin of the particle. Recognizing that the problem is a degenerate perturbation theory problem tells us that we need to use the following method:

For first-order time-independent *degenerate* perturbation theory problems, diagonalize the matrix $\langle n^{(i)} | V | n^{(j)} \rangle$. Here, V is the perturbation Hamiltonian. $|n^{(i)}\rangle$ is a basis vector of the degenerate subspace of eigenvectors of the unperturbed Hamiltonian H_0 that have energy E_n.
The eigenvalues of $\langle n^{(i)} | V | n^{(j)} \rangle$ are the energy shifts (to first order) caused by the perturbation V.
The eigenvectors of $\langle n^{(i)} | V | n^{(j)} \rangle$ are the lowest-order perturbative approximation of the eigenstates of the full Hamiltonian $H_0 + V$.

Here, the perturbation Hamiltonian is given by the problem statement:

$$V(x) = \mu_0 \boldsymbol{\sigma} \cdot \mathbf{B} = \begin{cases} \mu_0 B \sigma_z & -L \le x \le 0 \\ \mu_0 B \sigma_x & 0 < x \le L \end{cases} \tag{71}$$

Note that V is piecewise constant, and it only depends on whether the particle is in the left half or the right half of the box. Since $V(x)$ only depends on whether the particle is in the left or right half of the box, we can simplify the spatial wavefunction of the particle:

$$|\psi\rangle = \ell\,|L\rangle + r\,|R\rangle \tag{72}$$

where $|L\rangle$ represents the particle being in the left side of the box and R represents the particle being in the right side of the box. Here, we have $\langle L|L\rangle = \langle R|R\rangle = 1$ and $\langle L|R\rangle = \langle R|L\rangle = 0$, since there is no overlap between the two states. Note also the following:

- Each of the energy eigenfunctions for the particle in a box $\psi_n(x)$ are either even or odd, as measured about the center of the box.
- The probability density of finding the particle in a location x is given by $|\psi_n(x)|^2$.
- Therefore, assuming the particle is in an energy eigenfuction for the infinite square well potential, the probability of finding the particle in the left half of the box is equal to the probability of finding the particle in the right half of the box.

Therefore, if $|\psi\rangle$ is an energy eigenstate of the unperturbed Hamiltonian (the one-dimensional infinite square well potential), we have

$$|\psi_n\rangle = \ell\,|L\rangle + r\,|R\rangle \quad \text{with} \quad |\ell|^2 = |r|^2 = \frac{1}{2} \tag{73}$$

since the particle is equally likely to be found in either side of the box.

The degenerate subspace of all states that have the same unperturbed energy E_n is just the set of all particles with spatial state given by $|\psi\rangle_n$ and different spin states. It is spanned by the vectors

$$|\psi_n,\uparrow\rangle = (\ell\,|L\rangle + r\,|R\rangle)\,|\uparrow\rangle \quad \text{and} \quad |\psi_n,\downarrow\rangle = (\ell\,|L\rangle + r\,|R\rangle)\,|\downarrow\rangle \tag{74}$$

The perturbation Hamiltonian (71) is equal to $\mu_0 B\sigma_z$ if the particle is in state $|L\rangle$, and it is equal to $\mu_0 B\sigma_x$ if the particle is in state $|R\rangle$. It does not change the spatial wavefunction of the particle. Therefore, we can write the perturbation Hamiltonian in Dirac notation as

$$V = \mu_0 B\Big(\,|L\rangle\,\sigma_z\,\langle L| + |R\rangle\,\sigma_x\,\langle R|\,\Big) \tag{75}$$

We can start to calculate the matrix elements of V. Let s_1 and s_2 be stand-ins for either spin-up $\uparrow$ or spin-down $\downarrow$. Then, by (75),

$$\begin{aligned} V\,|\psi_n, s_2\rangle &= \mu_0 B\Big(\,|L\rangle\,\sigma_z\,\langle L| + |R\rangle\,\sigma_x\,\langle R|\,\Big)\,(\ell\,|L\rangle + r\,|R\rangle)\,|s_2\rangle \\ &= \mu_0 B\Big(\ell\,|L\rangle\,\sigma_z\,|s_2\rangle + r\,|R\rangle\,\sigma_x\,|s_2\rangle\Big) \quad \text{as } \langle L|L\rangle = \langle R|R\rangle = 1 \text{ and } \langle L|R\rangle = 0 \end{aligned} \tag{76}$$

Taking the inner product of these states with the basis state $|\psi_n, s_1\rangle$, we get

$$\begin{aligned} \langle\psi_n, s_1|V|\psi_n, s_2\rangle &= \mu_0 B\Big(\ell^*\,\langle L| + r^*\,\langle R|\Big)\,\langle s_1|\cdot\Big(\ell\,|L\rangle\,\sigma_z\,|s_2\rangle + r\,|R\rangle\,\sigma_x\,|s_2\rangle\Big) \\ &= \mu_0 B\Big(\ell^*\ell\,\langle s_1|\sigma_z|s_2\rangle + r^*r\,\langle s_1|\sigma_x|s_2\rangle\Big) \quad \text{as } \langle L|L\rangle = \langle R|R\rangle = 1 \text{ and } \langle L|R\rangle = 0 \\ &= \frac{\mu_0 B}{2}\,(\,\langle s_1|\sigma_z|s_2\rangle + \,\langle s_1|\sigma_x|s_2\rangle) \quad \text{since } \ell^*\ell = |\ell|^2 = \frac{1}{2} \text{ and } r^*r = |r|^2 = \frac{1}{2} \end{aligned} \tag{77}$$

The matrix elements $\langle s_1|\sigma_z|s_2\rangle$ and $\langle s_1|\sigma_x|s_2\rangle$ are just elements of the Pauli matrices, as they act on the spinors $\begin{pmatrix} a \\ b \end{pmatrix} \cong a\,|{\uparrow}\rangle + b\,|{\downarrow}\rangle$ Putting all of this together, we can write the restriction of V to the degenerate subspace spanned by $|\psi_n, {\uparrow}\rangle$ and $|\psi_n, {\downarrow}\rangle$ in matrix form:

$$
\begin{aligned}
V &\cong \begin{pmatrix} \langle\psi_n,{\uparrow}|V|\psi_n,{\uparrow}\rangle & \langle\psi_n,{\uparrow}|V|\psi_n,{\downarrow}\rangle \\ \langle\psi_n,{\downarrow}|V|\psi_n,{\uparrow}\rangle & \langle\psi_n,{\downarrow}|V|\psi_n,{\downarrow}\rangle \end{pmatrix} \\
&= \frac{\mu_0 B}{2}\left[\begin{pmatrix} \langle{\uparrow}|\sigma_z|{\uparrow}\rangle & \langle{\uparrow}|\sigma_z|{\downarrow}\rangle \\ \langle{\downarrow}|\sigma_z|{\uparrow}\rangle & \langle{\downarrow}|\sigma_z|{\downarrow}\rangle \end{pmatrix} + \begin{pmatrix} \langle{\uparrow}|\sigma_x|{\uparrow}\rangle & \langle{\uparrow}|\sigma_x|{\downarrow}\rangle \\ \langle{\downarrow}|\sigma_x|{\uparrow}\rangle & \langle{\downarrow}|\sigma_x|{\downarrow}\rangle \end{pmatrix}\right] \quad \text{by (77)} \\
&= \frac{\mu_0 B}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] \quad \text{by definition of the Pauli matrices} \\
&= \frac{\mu_0 B}{2} A \quad \text{for} \quad A \equiv \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}
\end{aligned} \tag{78}
$$

The eigenvalues of V are the first-order energy shifts under the perturbation. To find the eigenvalues of V, set the characteristic polynomial of the matrix $A \equiv \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ equal to zero:

$$
\begin{aligned}
0 &= \det(A - \lambda I) \\
&= \det\begin{pmatrix} 1-\lambda & 1 \\ 1 & -1-\lambda \end{pmatrix} \\
&= (1-\lambda)(-1-\lambda) - (1)(1) \\
&= \left(\lambda^2 - 1\right) - 1 \\
0 &= \lambda^2 - 2
\end{aligned} \tag{79}
$$

The solutions of this equation, the eigenvalues of A, are given by

$$\lambda_\pm = \pm\sqrt{2} \tag{80}$$

V is just equal to $\mu_0 B/2$ times A, so the eigenvalues of V are equal to

$$
\begin{aligned}
\Delta E_\pm &= \frac{\mu_0 B}{2}\lambda_\pm \\
&= \frac{\mu_0 B}{2}\left(\pm\sqrt{2}\right) \\
\Delta E_\pm &= \pm\frac{\mu_0 B}{\sqrt{2}}
\end{aligned} \tag{81}
$$

All that remains is to add the unperturbed energy levels E_n to the energy shifts $\Delta E_\pm$. Using (70) and bearing in mind that the box is of width $2L$, not L, we get that the unperturbed energy levels are

$$E_n = \frac{\hbar^2\pi^2 n^2}{2m(2L)^2} = \frac{\hbar^2\pi^2 n^2}{8mL^2} \quad \text{for} \quad n = 1, 2, 3, \ldots \tag{82}$$

Therefore, the energy levels of the particle to first order in B are

$$\boxed{E_{n,\pm} = \frac{\hbar^2\pi^2 n^2}{8mL^2} \pm \frac{\mu_0 B}{\sqrt{2}} \quad \text{for} \quad n = 1, 2, 3, \ldots} \tag{83}$$

Above, we used the kets $|L\rangle$ and $|R\rangle$ to represent which side of the box the particle is in. This approach doesn't require us to know the precise form of the particle-in-a-box wavefunctions—just the fact that each wavefunction is either even or odd—and it doesn't require us to take any integrals.

It is instructive, though, to demonstrate how to derive the matrix elements in (78) using the exact wavefunctions of the particle in a box. Recall that the wavefunctions of the particle in a box are the sine and cosine functions that are equal to zero at both sides of the box (in this case, $x = \pm L$). Since the box is of width $2L$, the allowed wavenumbers are $k_n = n\pi/(2L)$. We know from the diagram above that the parity of each eigenfunction ψ_n is the opposite of the parity of n (so the $n = 1$ eigenfunction is a cosine function, the $n = 2$ eigenfunction is a sine function, and so on). From this information, we can read off the eigenfunctions:

$$\psi_n(x) = \begin{cases} N_n \cos\left(\frac{n\pi x}{2L}\right) & \text{for} \quad n = 1, 3, 5, \dots \\ N_n \sin\left(\frac{n\pi x}{2L}\right) & \text{for} \quad n = 2, 4, 6, \dots \end{cases} \tag{84}$$

Here, the normalization constant N_n is defined so that

$$\int_{-L}^{L} dx \; |\psi_n(x)|^2 = 1 \tag{85}$$

With this information, we can find the matrix elements of V. Using (71)

$$V(x) = \begin{cases} \mu_0 B \sigma_z & -L \le x \le 0 \\ \mu_0 B \sigma_x & 0 < x \le L \end{cases}$$

we can write (where s_1 and s_2 are stand-ins for either spin-up or spin-down)

$$\begin{aligned} \langle \psi_n, s_1 | V | \psi_n, s_2 \rangle &= \int_{-L}^{L} dx \left(\psi_n^*(x) \langle s_1 | \right) V(x) \left(\psi_n(x) | s_2 \rangle \right) \\ &= \int_{-L}^{0} dx \, \psi_n^*(x) \langle s_1 | V(x) \psi_n(x) | s_2 \rangle + \int_{0}^{L} dx \, \psi_n^*(x) \langle s_1 | V(x) \psi_n(x) | s_2 \rangle \\ &= \mu_0 B \left[\int_{-L}^{0} dx \, \psi_n^*(x) \langle s_1 | \sigma_z \psi_n(x) | s_2 \rangle + \int_{0}^{L} dx \, \psi_n^*(x) \langle s_1 | \sigma_x \psi_n(x) | s_2 \rangle \right] \end{aligned}$$

Since σ_z does not act on the spatial component of the wavefunction, we can pull $\psi_n(x)$ out of the spin matrix element and combine it with its conjugate $\psi_n^*(x)$ to get $|\psi_n(x)|^2$:

$$\langle \psi_n, s_1 | V | \psi_n, s_2 \rangle = \mu_0 B \left[\int_{-L}^{0} dx \; |\psi_n(x)|^2 \langle s_1 | \sigma_z | s_2 \rangle + \int_{0}^{L} dx \; |\psi_n(x)|^2 \langle s_1 | \sigma_x | s_2 \rangle \right]$$

$\langle s_1 | \sigma_i | s_2 \rangle$ is just the matrix element of the Pauli matrix σ_i. This gets us to

$$\langle \psi_n, s_1 | V | \psi_n, s_2 \rangle = \mu_0 B \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \int_{-L}^{0} dx \; |\psi_n(x)|^2 + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \int_{0}^{L} dx \; |\psi_n(x)|^2 \right] \tag{86}$$

where the matrices act on a spinor $\begin{pmatrix} a \\ b \end{pmatrix} \cong a |\uparrow\rangle + b |\downarrow\rangle$. Since $\psi_n(x)$ is either even (a cosine function) or odd (a sine function), we must have

$$|\psi_n(-x)|^2 = |\pm \psi_n(x)|^2 = |\psi_n(x)|^2 \tag{87}$$

so $|\psi_n(x)|^2$ is an even function. Using information about the integral of an even function, we get

$$\begin{aligned} \int_{-L}^{0} dx \; |\psi_n(x)|^2 = \int_{0}^{L} dx \; |\psi_n(x)|^2 &= \frac{1}{2} \int_{-L}^{L} dx \; |\psi_n(x)|^2 \\ &= \frac{1}{2} \quad \text{by the normalization} \int_{-L}^{L} dx \; |\psi_n(x)|^2 = 1 \end{aligned} \tag{88}$$

Plugging this into (86), we get the same result as when we used the kets $|L\rangle$, $|R\rangle$:

$$\langle \psi_n, s_1 | V | \psi_n, s_2 \rangle = \frac{\mu_0 B}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] = \frac{\mu_0 B}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{89}$$

The rest of the calculation proceeds as before.